

AD-A168 924

CALCULATED VERSUS EXPERIMENTAL CHARGE DENSITY
DISTRIBUTION OF BE METAL(U) CORNELL UNIV ITHACA NY LAB
OF ATOMIC AND SOLID STATE PHYSICS.. A J PINDOR ET AL.

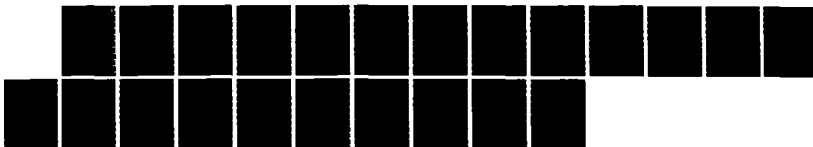
1/1

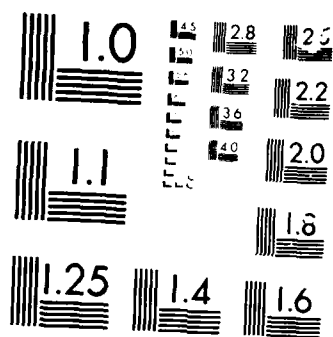
UNCLASSIFIED

JUN 86 TR-23 N00014-82-K-0576

F/G 20/0

NL





MICROGRAPH

10-11

AD-A168 924

OFFICE OF NAVAL RESEARCH

Contract N00014-82-K-0576

TECHNICAL REPORT NO. 23

CALCULATED VS. EXPERIMENTAL CHARGE

DENSITY DISTRIBUTION OF BE METAL

by

A.J. Pindor, S.H. Vosko and C.J. Unrigar

Prepared for Publication

in

Journal of Physics F

University of Toronto
Department of Physics
Toronto, Ontario
M5S 1A7, Canada

and

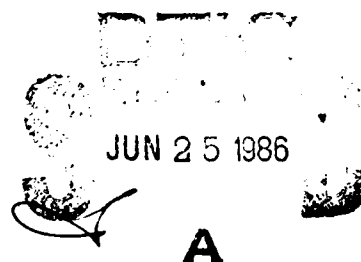
Laboratory of Atomic and Solid State Physics
Cornell University
Ithaca, New York 14853

June, 1986

Reproduction in whole or in part is permitted
for any purpose of the United States Government

This document has been approved for public release
and sale; its distribution is unlimited

DTIC FILE COPY



86 6 25 010

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER 23	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) CALCULATED VS. EXPERIMENTAL CHARGE DENSITY DISTRIBUTION OF BE METAL		5. TYPE OF REPORT & PERIOD COVERED Technical Report
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) A. J. Pindor and S. H. Vosko and C.J. Unrigar		8. CONTRACT OR GRANT NUMBER(s) N00014-82-K-0576
9. PERFORMING ORGANIZATION NAME AND ADDRESS LASSP, Cornell University, Ithaca, NY 14853 Department of Physics, University of Toronto Toronto, Ontario, M5S 1A7, Canada		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research 800 N. Quincy St. Arlington, VA 22217		12. REPORT DATE June, 1986-
		13. NUMBER OF PAGES 19
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) This document has been approved for public release and sale; its distribution unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES Submitted for publication in Journal of Physics F		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number)		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) We have performed self-consistent Linearized Augmented Plane Wave calculations of the charge density of metallic beryllium, with and without warping of the interstitial potential, using the Local Density Approximation for the exchange and correlation energy functional. Overall agreement with the newest x-ray form factors is good, and it is argued that the remaining discrepancies have their source in the inadequacy of the Local Density Approximation and, for some reflections, in neglecting the non-sphericity of the core charge density.		

1. CALCULATED VS. EXPERIMENTAL CHARGE DENSITY DISTRIBUTION
OF BE METAL

A.J.Pindor, S.H.Vosko

Department of Physics, University of Toronto,
Toronto, Ontario, M5S 1A7, Canada

and

C.J.Umrigar

Laboratory of Atomic and Solid State Physics,
Cornell University, Ithaca, NY, 14853, USA

Short title: Electronic charge density of Be metal

Classification number : 71.25P

Association For	
1955-1956	X
1957-1958	
1959-1960	
1961-1962	
1963-1964	
1965-1966	
1967-1968	
1969-1970	
1971-1972	
1973-1974	
1975-1976	
1977-1978	
1979-1980	
1981-1982	
1983-1984	
1985-1986	
1987-1988	
1989-1990	
1991-1992	
1993-1994	
1995-1996	
1997-1998	
1999-2000	
2001-2002	
2003-2004	
2005-2006	
2007-2008	
2009-2010	
2011-2012	
2013-2014	
2015-2016	
2017-2018	
2019-2020	
2021-2022	
2023-2024	
2025-2026	
2027-2028	
2029-2030	
2031-2032	
2033-2034	
2035-2036	
2037-2038	
2039-2040	
2041-2042	
2043-2044	
2045-2046	
2047-2048	
2049-2050	
2051-2052	
2053-2054	
2055-2056	
2057-2058	
2059-2060	
2061-2062	
2063-2064	
2065-2066	
2067-2068	
2069-2070	
2071-2072	
2073-2074	
2075-2076	
2077-2078	
2079-2080	
2081-2082	
2083-2084	
2085-2086	
2087-2088	
2089-2090	
2091-2092	
2093-2094	
2095-2096	
2097-2098	
2099-2100	
2101-2102	
2103-2104	
2105-2106	
2107-2108	
2109-2110	
2111-2112	
2113-2114	
2115-2116	
2117-2118	
2119-2120	
2121-2122	
2123-2124	
2125-2126	
2127-2128	
2129-2130	
2131-2132	
2133-2134	
2135-2136	
2137-2138	
2139-2140	
2141-2142	
2143-2144	
2145-2146	
2147-2148	
2149-2150	
2151-2152	
2153-2154	
2155-2156	
2157-2158	
2159-2160	
2161-2162	
2163-2164	
2165-2166	
2167-2168	
2169-2170	
2171-2172	
2173-2174	
2175-2176	
2177-2178	
2179-2180	
2181-2182	
2183-2184	
2185-2186	
2187-2188	
2189-2190	
2191-2192	
2193-2194	
2195-2196	
2197-2198	
2199-2200	
2201-2202	
2203-2204	
2205-2206	
2207-2208	
2209-2210	
2211-2212	
2213-2214	
2215-2216	
2217-2218	
2219-2220	
2221-2222	
2223-2224	
2225-2226	
2227-2228	
2229-2230	
2231-2232	
2233-2234	
2235-2236	
2237-2238	
2239-2240	
2241-2242	
2243-2244	
2245-2246	
2247-2248	
2249-2250	
2251-2252	
2253-2254	
2255-2256	
2257-2258	
2259-2260	
2261-2262	
2263-2264	
2265-2266	
2267-2268	
2269-2270	
2271-2272	
2273-2274	
2275-2276	
2277-2278	
2279-2280	
2281-2282	
2283-2284	
2285-2286	
2287-2288	
2289-2290	
2291-2292	
2293-2294	
2295-2296	
2297-2298	
2299-2300	
2301-2302	
2303-2304	
2305-2306	
2307-2308	
2309-2310	
2311-2312	
2313-2314	
2315-2316	
2317-2318	
2319-2320	
2321-2322	
2323-2324	
2325-2326	
2327-2328	
2329-2330	
2331-2332	
2333-2334	
2335-2336	
2337-2338	
2339-2340	
2341-2342	
2343-2344	
2345-2346	
2347-2348	
2349-2350	
2351-2352	
2353-2354	
2355-2356	
2357-2358	
2359-2360	
2361-2362	
2363-2364	
2365-2366	
2367-2368	
2369-2370	
2371-2372	
2373-2374	
2375-2376	
2377-2378	
2379-2380	
2381-2382	
2383-2384	
2385-2386	
2387-2388	
2389-2390	
2391-2392	
2393-2394	
2395-2396	
2397-2398	
2399-2400	
2401-2402	
2403-2404	
2405-2406	
2407-2408	
2409-2410	
2411-2412	
2413-2414	
2415-2416	
2417-2418	
2419-2420	
2421-2422	
2423-2424	
2425-2426	
2427-2428	
2429-2430	
2431-2432	
2433-2434	
2435-2436	
2437-2438	
2439-2440	
2441-2442	
2443-2444	
2445-2446	
2447-2448	
2449-2450	
2451-2452	
2453-2454	
2455-2456	
2457-2458	
2459-2460	
2461-2462	
2463-2464	
2465-2466	
2467-2468	
2469-2470	
2471-2472	
2473-2474	
2475-2476	
2477-2478	
2479-2480	
2481-2482	
2483-2484	
2485-2486	
2487-2488	
2489-2490	
2491-2492	
2493-2494	
2495-2496	
2497-2498	
2499-2500	
2501-2502	
2503-2504	
2505-2506	
2507-2508	
2509-2510	
2511-2512	
2513-2514	
2515-2516	
2517-2518	
2519-2520	
2521-2522	
2523-2524	
2525-2526	
2527-2528	
2529-2530	
2531-2532	
2533-2534	
2535-2536	
2537-2538	
2539-2540	
2541-2542	
2543-2544	
2545-2546	
2547-2548	
2549-2550	
2551-2552	
2553-2554	
2555-2556	
2557-2558	
2559-2560	
2561-2562	
2563-2564	
2565-2566	
2567-2568	
2569-2570	
2571-2572	
2573-2574	
2575-2576	
2577-2578	
2579-2580	
2581-2582	
2583-2584	
2585-2586	
2587-2588	
2589-2590	
2591-2592	
2593-2594	
2595-2596	
2597-2598	
2599-2600	
2601-2602	
2603-2604	
2605-2606	
2607-2608	
2609-2610	
2611-2612	
2613-2614	
2615-2616	
2617-2618	
2619-2620	
2621-2622	
2623-2624	
2625-2626	
2627-2628	
2629-2630	
2631-2632	
2633-2634	
2635-2636	
2637-2638	
2639-2640	
2641-2642	
2643-2644	
2645-2646	
2647-2648	
2649-2650	
2651-2652	
2653-2654	
2655-2656	
2657-2658	
2659-2660	
2661-2662	
2663-2664	
2665-2666	
2667-2668	
2669-2670	
2671-2672	
2673-2674	
2675-2676	
2677-2678	
2679-2680	
2681-2682	
2683-2684	
2685-2686	
2687-2688	
2689-2690	
2691-2692	
2693-2694	
2695-2696	
2697-2698	
2699-2700	
2701-2702	
2703-2704	
2705-2706	
2707-2708	
2709-2710	
2711-2712	
2713-2714	
2715-2716	
2717-2718	
2719-2720	
2721-2722	
2723-2724	
2725-2726	
2727-2728	
2729-2730	
2731-2732	
2733-2734	
2735-2736	
2737-2738	
2739-2740	
2741-2742	
2743-2744	
2745-2746	
2747-2748	
2749-2750	
2751-2752	
2753-2754	
2755-2756	
2757-2758	
2759-2760	
2761-2762	
2763-2764	
2765-2766	
2767-2768	
2769-2770	
2771-2772	
2773-2774	
2775-2776	
2777-2778	
2779-2780	
2781-2782	
2783-2784	
2785-2786	
2787-2788	
2789-2790	
2791-2792	
2793-2794	
2795-2796	
2797-2798	
2799-2800	
2801-2802	
2803-2804	
2805-2806	
2807-2808	
2809-2810	
2811-2812	
2813-2814	
2815-2816	
2817-2818	
2819-2820	
2821-2822	
2823-2824	
2825-2826	
2827-2828	
2829-2830	
2831-2832	
2833-2834	
2835-2836	
2837-2838	
2839-2840	
2841-2842	
2843-2844	
2845-2846	
2847-2848	
2849-2850	
2851-2852	
2853-2854	
2855-2856	
2857-2858	
2859-2860	
2861-2862	
2863-2864	
2865-2866	
2867-2868	
2869-2870	
2871-2872	
2873-2874	
2875-2876	
2877-2878	
2879-2880	
2881-2882	
2883-2884	
2885-2886	
2887-2888	
2889-2890	
2891-2892	
2893-2894	
2895-2896	
2897-2898	
2899-2900	
2901-2902	
2903-2904	
2905-2906	
2907-2908	
2909-2910	
2911-2912	
2913-2914	
2915-2916	
2917-2918	
2919-2920	
2921-2922	
2923-2924	
2925-2926	
2927-2928	
2929-2930	
2931-2932	
2933-2934	
2935-2936	
2937-2938	
2939-2940	
2941-2942	
2943-2944	
2945-2946	
2947-2948	
2949-2950	
2951-2952	
2953-2954	
2955-2956	
2957-2958	
2959-2960	
2961-2962	
2963-2964	
2965-2966	
2967-2968	
2969-2970	
2971-2972	
2973-2974	
2975-2976	
2977-2978	
2979-2980	
2981-2982	
2983-2984	
2985-2986	
2987-2988	
2989-2990	
2991-2992	
2993-2994	
2995-2996	
2997-2998	
2999-3000	

A-1



A B S T R A C T

We have performed self-consistent Linearized Augmented Plane Wave calculations of the charge density of metallic beryllium, with and without warping of the interstitial potential, using the Local Density Approximation for the exchange and correlation energy functional. Overall agreement with the newest x-ray form factors is good, and it is argued that the remaining discrepancies have their source in the inadequacy of the Local Density Approximation and, for some reflections, in neglecting the non-sphericity of the core charge density.

1. INTRODUCTION

Recently very careful measurements of the X-ray structure factors for Be metal have become available (Hansen et al 1984). Since the X-ray structure factors are directly related to the electron charge density, which in principle is exactly calculable from Density Functional Theory (DFT), these results can be used as a stringent test of present day practice of DFT i.e. the Local Density Approximation (LDA) for the exchange and correlation energy functional (for recent reviews see Theory of Inhomogeneous Electron Gas, ed. S. Lundqvist and N.H. March, Plenum Press, New York, 1983). In fact the X-ray structure factors provide a more severe test of LDA than its very successful application to the calculation of such physical quantities as cohesive energies, compressibilities, lattice constants etc., which are obtained from total energy differences where substantial cancellation of errors can occur (see Morrucci et al. 1978). No such cancellation of errors takes place in the calculation of the structure factors.

It is important to be aware that in the practical implementation of DFT there are two distinct sources for the discrepancies between theory and experiment. One, which may be termed as fundamental, is due to the fact that the exact exchange-correlation energy functional is unknown. As in

most current applications, the Local Density Approximation (LDA) (see eg. Williams and von Barth, 1983) is used in the present work (specifically the standard form for exchange with the Vosko et al. (1980), hereafter referred to as VWN, form for the correlation part). The second comes from the computational aspect of the problem, namely the numerical solution of the self-consistent Kohn-Sham equations for the Belectrons in a crystal, for which a number of approximations must be made. Although in principle these are controllable, increasing the accuracy of the results puts rapidly growing demands on the necessary computer resources. In the present case we only require that the degree of self-consistency be such that the errors in the calculated form factors be less than the experimental ones.

To investigate the effects of the metallic environment on the charge redistribution in Be, we have performed Linearized Augmented Plane Wave (LAPW) calculations for the valence electrons, with and without warping of the interstitial potential. The 1s electrons were treated as atomic-like, since they had totally negligible amount of charge in the interstitial region (less than 0.001 of an electron). However, they were not frozen, i.e. their wave functions were recalculated at each iteration step.

We have used experimental lattice constants: $a = 4.3211$ and $c = 6.7715$ a.u. The resulting Fourier components of the charge density compare favourably with experimental data, as discussed below. However, a number of discrepancies remain. We argue, by reference to atomic LDA, Hartree-Fock (H-F) and Configuration Interaction (CI) charge densities, that the discrepancies for high Fourier components of the charge density are due to inadequacy of LDA to describe electron-electron interaction in the core region, where electron density gradients are large. We also expect that an appreciable discrepancy for the second Fourier component is due to the fact that we have not taken into account properly the distortion of the $1s$ core caused by the metallic environment.

2. OVERLAPPING ATOMIC CHARGE DENSITIES

As a first step we calculate the form factors for the density distribution corresponding to overlapping Be atomic electron densities obtained using different treatments of many-body effects. The intention is to calibrate the LDA with respect to more exact treatments (i.e. CI, which we consider virtually exact, and H-F), to have a reference system from which to measure metallization effects and

finally to have an estimate of the relative importance of core versus valence electron contributions to the form factors.

The results are summarized in Table I. The third column gives form factors obtained using atomic charge densities from a CI calculation using 55 configurations (Boyd 1979), the fourth column presents results from LDA, and the fifth - H-F calculation using Clementi and Roetti (1974) wave functions. For H-F results we also show separately the contribution from the 2s (valence) electrons. Finally column two shows the experimental results of Hansen et al.(1984), corrected for effects of atomic vibrations (Larsen et al 1980), together with estimated errors.

From a comparison of the three theoretical columns it can be seen that the H-F values are much closer to the "exact" CI values than the LDA ones. This is in agreement with previous observations that the local treatment of exchange is a more important source of error in the charge density than the neglect of correlation (Vosko and Wilk 1983). Moreover, the difference between H-F and CI is of the order or less than the experimental uncertainty, suggesting that if one could perform a calculation for the metal equivalent to H-F (e.g. essentially exact treatment of exchange within DFT) the error would be much smaller than

the experimental error and the main source of error would be in the accuracy of solving the Kohn-Sham equations..

Comparing CI and the experimental results for the individual wave vectors one sees that in most cases they differ by more than the uncertainty in the measurements indicating the necessity of including the effects of the crystal environment. On the other hand the magnitude of the differences generally decreases with increasing length of wave vector, as expected, since crystal field effects are smaller in the vicinity of the nucleus, which becomes more important as the order of reflection increases. However, since the LDA is used in the metallic calculation, it is also important to note that the magnitude of the percentage difference between the atomic CI and LDA calculations increases from $\sim 0.5\%$ to $\sim 1\%$ as the order of reflection increases. Thus we expect the difference in the LDA metallic calculation and experiment to increase with the magnitude of the wave vector. This is in fact what occurs as can be seen from Table II.

The other fact we would like to point out is that the contribution of the 2s states is only 1-2% of the total. Thus even though we expect the effect of the metallic environment on the core states to be small, it can have an appreciable influence on the change of form factors on

going from atom to metal, since the contribution from the core is the dominant part of the total form factor.

3. LAPW FORM FACTORS.

3.1 Computational details

To study effects of metallization on the electronic charge distribution we have performed self-consistent, warped muffin-tin, LAPW band structure calculations (see e.g. Andersen 1975, Koelling and Arbman 1975), with the VWN form of LDA. Basis functions inside the muffin-tin included angular momentum components up to $\ell=8$ and in the interstitial region we found it necessary to go to over 50 plane waves, i.e. to take $k_{\max} \cdot R_{\text{MT}} = 6.4$. Increasing $k_{\max} \cdot R_{\text{MT}}$ to 7.5 did not modify the results in a significant way. The energy parameter was chosen in the middle of the band, $E=0.4$ Ry. Brillouin zone integrations were performed using the special points method (Fehlner and Vosko 1977), and we used as a standard 35 points in the irreducible part of the B.Z. Increasing this number to 57 had only a minor effect on the form factors. Nonsphericity of the valence charge density inside the muffin-tin was taken into account only approximately by analytically continuing the non-spherical part of the interstitial charge density into the

MT spheres. Since the non-sphericity is large only near the MT boundary this procedure yields a good approximation to the non-spherical part of the valence charge density. However this procedure cannot be used for the core charge density since so little of the core charge (less than 0.001 of an electron) is in the interstitial region that an analytic continuation would be unreliable. Hence we have not included the non-sphericity of the core charge. However the core charge was not frozen, i.e. the core wavefunctions were recalculated at each iteration step. The neglect of the small non-sphericity of the core charge is normally of no consequence but in the present calculation it is because no less than 96% of the form factors comes from the core charge and we are interested in the small changes in the form factors that occur on forming a solid. Hence we expect that possible discrepancies between our calculated form factors and the experimental ones will be due to the neglect of the core charge distortion and/or to inadequacy of LDA.

3.2 Results

Table II presents results of our calculations (warped and MT) and for comparison we also show results obtained by Chen et al. (1988) using the self-consistent

pseudopotential method. The MT calculation was performed to investigate the importance of "warping" of the interstitial potential on the charge density. For the low order beams (with the exception of 002) the warped calculation agrees better with experiment than the atomic calculations. Warping is important for obtaining agreement for the lowest order reflection but affects the other reflections only slightly. The disagreement in the 002 form factor is probably due to our neglect of the non-sphericity of the core. Since the c/a ratio (1.57) for Be metal is appreciably different from that for an ideal hcp crystal (1.63) it is likely that the core charge would be more non-spherical than in a close-packed structure. The 002 component is sensitive only to distortions in the z direction.

Table III compares the form factors of the core charge density from our self-consistent calculations with those for a free Be atom using the VWN form of LDA. The difference between these form factors is shown in the fourth column and the difference divided by the corresponding geometric structure factor in the fifth column. The entries in the fifth column are all positive and increase with the magnitude of $\sin\theta/\lambda$, indicating an expansion of the cores in the metallic environment as expected.

The values of the last three form factors obtained from the warped calculation are all appreciably smaller than the experimental values. This is probably due to the inadequacy of LDA when the gradients of the charge density are large.

The LDA is known to give much better results when used to calculate differences of various quantities than their absolute values. We can crudely include both the effects of metallization and non-local effects in the exchange correlation potential by recasting our results in terms of a difference in the two LDA calculations plus the CI form factor (using H-F atomic form factor, if CI was not available, would also be adequate):

$$f_D = f_{LDA}^{(met)} - f_{LDA}^{(at)} + f_{CI}^{(at)} \quad (1)$$

where $f_{LDA}^{(met)}$ is our calculated form factor for the metal (column 2 of Table II), $f_{LDA}^{(at)}$ is atomic form factor (column 4 of Table I) - both calculated within LDA and $f_{CI}^{(at)}$ is the CI atomic form factor (column 3 of Table I). We see that in general we get an improvement, with the exception of the 002 reflection, which becomes worse. This again suggests that it is distortion of the cores due to the metallic environment, which is a source of the discrepancy in this case.

4. CONCLUSIONS

In conclusion we state that metallization effects are important for obtaining agreement of theoretical short wave vector Fourier components of charge density in metallic Be with recent accurate experimental data. In particular, for the shortest component inclusion of warping of the interstitial potential is essential. For higher q components the LDA seems to become less adequate, which is not surprising since such Fourier components are sensitive to the charge distribution in the core region where gradients of the charge density are large and hence corrections to LDA are expected to be substantial. We also note that the contribution from valence electrons constitutes less than 4% of the total value of the form factors (and this fraction goes down with increasing q) and hence even a small distortion of the core wave functions may contribute significantly to the form factors. We expect that this effect, not taken into account in our calculations, is responsible for marked disagreement between our calculated and experimental values for the 002 form factor.

5. ACKNOWLEDGMENTS

We thank Prof. R.J. Boyd for providing unpublished results of CI calculations.

This work was supported in part by a grant from the Natural Science and Engineering Council of Canada. CJU acknowledges the support of the Office of Naval Research.

REFERENCES

- Andersen O K 1975 Phys Rev B12 3060-3070
- Boyd R J 1979 private communication
- Chou M Y Lam P K and Cohen M L 1983 Phys Rev B28 4179-4185
- Clementi E and Roetti C 1974 At Data Nucl Data Tables 14 177
- Fehlner W R and Vosko S H 1977 Can J Physics 55 2041-2058
- Hansen N K and Schneider J R Larsen F K 1984 Phys Rev B29 917-926
- Koelling D D and Arbman G O 1975 J Phys F: Metal Physics 5 2041-2054
- Larsen F K Lehmann M S and Merisolo M 1980 Acta Crystal Sect A36 159
- Moruzzi V L Janak J F Williams A R 1978 Calculated electronic properties of metals Pergamon Press Inc.
- Vosko S H and Wilk L 1983 J Phys B: At Mol Phys 16 3687-3702
- Vosko S H Wilk L and Nusair M 1980 Can J Phys 58 1200
- Williams A R and von Barth U 1983 Theory of the Inhomogeneous Electron Gas ed Lundqvist S and March N H Plenum Press New York pp 189-308

TABLE CAPTIONS

Table I

Form factors of overlapping atomic charge densities for Be, calculated within different approximations:

CI - Configuration interaction with 55 configurations (Boyd 1979;)

LDA - Local Density Approximation in VWN form (Vosko et al 1980);

H-F - Hartree-Fock using Clementi and Roetti (1974) wave functions;

H-F 2s (column 6) is the contribution from H-F wave function. Experimental data are from Hansen et al.(1984)

Table II

Form factors of charge density for metallic beryllium. Columns 2 and 3 show our LAPW results with (warped) and without (MT) warping of the interstitial potential. For comparison we also show the results of Chou et al.(1983) in

column 4. Experimental data are from Hansen et al. (1984).
Column 6 gives the values of the quantity f_D defined in the
eq. 1.

Table III

Structure factors of the core charge density for Be. The
second column gives values obtained in our "warped" LAPW
calculation, the third column refers to the LDA atomic
calculation, the fourth column is the difference of the
previous two and in the last one we give this difference
divided by the geometric structure factor (GSF).

T A B L E I

hkl	Exp.	CI	LDA	H-F	H-F 2s
100	1.889(6)	1.826	1.817	1.818	0.020
002	3.432(7)	3.491	3.473	3.482	-0.034
101	2.938(7)	2.981	2.966	2.975	-0.044
102	1.550(11)	1.556	1.545	1.557	-0.036
110	2.909(18)	2.921	2.895	2.924	-0.036
103	2.406(12)	2.387	2.363	2.391	-0.006
200	1.368(7)	1.351	1.337	1.353	0.002
004	2.506(10)	2.527	2.497	2.531	0.024

T A B L E I I

hkl	Present calc.		Chou et al	Exp.	f_D
	warped	MT			
100	1.886	1.846	1.8845	1.889(6)	1.895
002	3.468	3.465	3.4418	3.432(7)	3.486
101	2.929	2.944	2.9255	2.938(7)	2.944
102	1.550	1.558	1.5365	1.550(11)	1.561
110	2.889	2.898	2.8669	2.909(18)	2.915
103	2.348	2.355	2.3362	2.406(12)	2.372
200	1.322	1.329	1.316	1.368(7)	1.336
004	2.470	2.478	2.4798	2.506(10)	2.500

T A B L E I I I

hkl	Metal ls	Atom ls	Atom-Metal	Atom-Metal/GSF
100	1.7873	1.7884	0.0011	0.0011
002	3.4901	3.4927	0.0026	0.0013
101	2.9955	2.9980	0.0025	0.0014
102	1.5729	1.5775	0.0022	0.0022
110	2.9142	2.9195	0.0053	0.0026
103	2.3524	2.3574	0.0050	0.0029
200	1.3273	1.3303	0.0030	0.0030
004	2.4541	2.4602	0.0061	0.0030

END

DTIC

7-86